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Exact and Improved Lattice Chiral Symmetry

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We present an overview of our quenched and dynamical tests of Wilson twisted mass fermions at full twist as a promising candidate for large scale numerical simulations to "solve" Quantum Chromodynamics.

1 Introduction

This project performed at the John von Neumann Institute for Computing aims at realistic simulations of our theory of strong interactions, Quantum Chromodynamics (QCD), on a 4-dimensional Euclidean lattice, where with "realistic" we mean the following: the three lightest –up, down, and strange– quarks should be taken as dynamical degrees of freedom in the simulation; the masses of these quarks should be tuned such that the experimentally observed values of the masses of the pion and the kaon are reproduced; the linear box length should be about $L = 3$fm, since, e.g. the diameter of the proton is about 1fm and it should fit comfortably; finally, the simulations have to be performed at a number of fine enough values of the lattice spacing a, i.e. $0.05\text{fm} \leq a \leq 0.1$fm in order to obtain a well controlled continuum extrapolation.

Unfortunately, the original formulation of lattice QCD by Wilson[1] has been found to possess some shortcomings which drive the above sketched realistic scenario very difficult, if not impossible with present and near future computer technology. The original Wilson lattice QCD formulation exhibits lattice spacing effects that are linear in the lattice spacing a and hence even a value of $a = 0.05$fm might not be sufficient to perform a controlled continuum extrapolation. Even more severely, although connected, this formulation breaks chiral symmetry[a] explicitly.

The *spontaneous* breaking of this chiral symmetry can explain the observed spectrum of light mesons and has important consequences for the understanding and interpretation of QCD. In particular, it is possible to write down an effective, low-energy theory of QCD, the so-called chiral perturbation theory Lagrangian, which relies on chiral symmetry and the mechanism of spontaneous chiral symmetry breaking and which has become a most important and powerful tool to analyze QCD phenomena at low energies[2,3].

2 New Lattice QCD Actions

The last years have seen a number of attempts to overcome the above mentioned difficulties of the original Wilson fermion action. In this project we have studied two of such formulations, the chiral invariant overlap fermions[4–7] and Wilson twisted mass fermions[8]. The

[a] Chiral symmetry is a symmetry of *continuum* QCD and means the invariance of the theory under the interchange of massless left- and right-handed fermions.

approach of chiral invariant formulations of lattice QCD has been discussed in a previous NIC proceedings contribution[9].

Unfortunately, the beauty of an exact lattice chiral symmetry comes with a rather high price of simulation cost which drives *dynamical* simulations with these kind of lattice fermions unrealistic presently. An alternative promising candidate are *maximally twisted Wilson fermions*[10,8]. This recent development adds a so-called twisted mass term $i\mu\gamma_5\tau_3$ to the usual Wilson Dirac operator. The action of twisted mass fermions then takes the form

$$S[U,\psi,\bar{\psi}] = a^4 \sum_x \bar{\psi}(x)(D_W + m_0 + i\mu\gamma_5\tau^3)\psi(x) \equiv \bar{\Psi} D_{\rm tm} \Psi \ . \tag{1}$$

Here, D_W is the standard, massless Wilson Dirac operator, m_0 is the bare quark mass parameter and μ the twisted mass parameter. Note that the Pauli-matrix τ_3 acts in flavour space. A first intriguing property of Wilson twisted mass fermions is that $\det[D_{\rm tm}] = \det[D_W(m_0)^2 + \mu^2]$. This determinant is regulated by the twisted mass parameter and cannot exhibit dangerously small or even negative eigenvalues as in the case of the standard Wilson Dirac operator. Note that the appearance of such very low-lying eigenvalues render dynamical simulations very costly, if not impossible.

A second, very remarkable property of Wilson twisted mass fermions is that they can be O(a) improved[b] without the need of additional improvement terms as they are needed for pure Wilson fermions[11,12]. The O(a)-improvement can be obtained by choosing the bare quark mass m_0 to assume a critical value $m_{\rm crit}$ which can be realized by searching for that value of m_0 where, e.g., the quark mass is zero[c].

The twisted mass fermion action of eq. (1) can be derived from the standard Wilson fermion action by performing an axial transformation on the fermion fields, i.e. $\psi \rightarrow e^{i\omega\gamma_5\tau^3/2}\psi$. This “twisting” of the fermion fields is maximal when $\omega = \pi/2$. Since the angle ω is related to the parameters m_0 and μ of eq. (1) by $\tan\omega = \mu/m$ with $m = m_0 - m_{\rm crit}$, maximal twist is obtained when $m_0 = m_{\rm crit}$ which was the condition for automatic O(a)-improvement. Another important aspect of Wilson twisted mass fermions in practice is that it reduces the unphysical mixing of operators[13,14]. Finally also non-degenerate quark masses can be realized, keeping the positivity of the fermionic determinant intact[14].

Given all these advertised advantages, our collaboration set out to investigate the potential of Wilson twisted mass fermions and test this new approach to lattice QCD. Our first aim was to see, whether Wilson twisted mass fermions are able to allow for simulations at considerably smaller pseudo scalar masses than with standard Wilson fermions[d]. Even more challenging is the question whether the values of pseudo scalar masses that are reachable with Wilson twisted mass fermions are comparable with those of chiral invariant overlap fermions.

The results of this first test of Wilson twisted mass fermions[15] is shown in fig. 1. This figure is a striking demonstration of the potential of Wilson twisted mass fermions. The smallest value of the pseudo scalar mass is basically identical with the one of overlap fermions and much smaller than the one from standard Wilson fermions.

A most intriguing question is, of course, whether one or the other formulation of lattice fermions does have an advantage in the computational cost. We have therefore explored

[b] In an O(a)-improved theory, the lattice spacing effects that appear linear in the lattice spacing are reduced and sometimes, as in the case of non-perturbative O(a)-improvement, even eliminated.
[c] Usually the so-called PCAC quark mass is taken for this purpose.
[d] We do not differentiate here whether original or non-perturbatively O(a)-improved Wilson fermions are used.

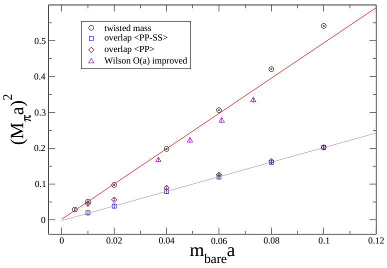

Figure 1. Comparison of quenched results for the pseudo scalar mass squared as a function of the bare quark mass for three lattice fermions: standard $\mathcal{O}(a)$ improved Wilson fermions, twisted mass fermions and overlap fermions.

V, m_π	Overlap	Wilson TM	rel. factor
12^4, 720Mev	48.8(6)	2.6(1)	18.8
12^4, 390Mev	142(2)	4.0(1)	35.4
16^4, 720Mev	225(2)	9.0(2)	25.0
16^4, 390Mev	653(6)	17.5(6)	37.3
16^4, 230Mev	1949(22)	22.1(8)	88.6

Table 1. The time in seconds on the NIC IBM JUMP machine to compute one propagator component using overlap or Wilson twisted mass fermions.

a large variety of algorithmic tricks to find the best and fastest way of computing one component of a fermion propagator with Wilson twisted mass and with overlap fermions[16]. The timing of these tests are listed in table 1 for a number of pseudo scalar mass values. Clearly, these results show that Wilson twisted mass fermions are at least one order of magnitude cheaper to simulate than overlap fermions while reaching similar small values of the pseudo scalar mass.

The next question is, whether Wilson twisted mass fermions indeed show the anticipated O(a)-improvement when m_0 is tuned to some $m_{\rm crit}$. That this is indeed the case can be seen in fig. 2[17–19]. Here we show the pion decay constant as a function of a^2 at a fixed, small pseudo scalar mass of $m_{\rm PS} \approx 280$MeV for two definitions of the critical quark mass m_0. For both definitions, the pion decay constant follows a linear behaviour in a^2, thus confirming that the lattice spacing effects that appear in O(a) are indeed canceled. The figure also illustrates that different definitions of $m_{\rm crit}$, although leading to O(a)-improvement, can have rather different strengths of the O(a^2) effects. Hence, the lesson from this is that care has to be taken to use an optimal definition of $m_{\rm crit}$. We remark that such an optimal definition is given by choosing the vanishing of the so-called PCAC quark as the value of $m_{\rm crit}$[19]. The effect of different choices of $m_{\rm crit}$ and the consequences on the $O(a^2)$ artefacts has been theoretically studied in chiral perturbation theory in refs.[20–22] and put on a more general ground in ref.[23].

In fig. 3 we show the *continuum* behaviour of the pion decay constant (left figure)[19] and the average momentum of a parton in a pion (right figure)[24]. Both graphs show that with Wilson twisted mass QCD the behaviour of physical observables can be studied as a

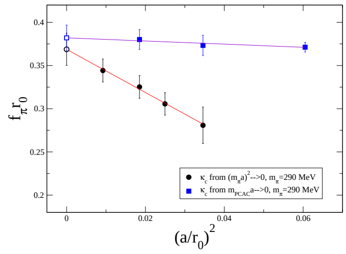

Figure 2. Scaling of the pseudo scalar decay constant f_π using two definitions of $m_{\rm crit}$ corresponding to two choices of κ_c.

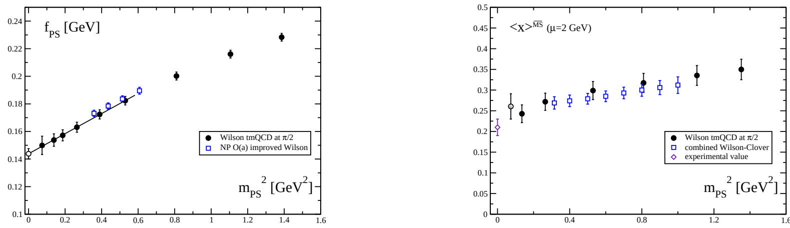

Figure 3. Continuum values of the pion decay constant (left) and the average momentum of a parton in a pion (right) as a function of the pseudo scalar mass in physical units.

function of the pseudo scalar mass down to small values below 300MeV *in the continuum*. It should be stressed that in principle even smaller values of the pseudo scalar mass could be reached and that it is only a question of computer resources to perform such simulations. Of course, in the here discussed quenched approximation it is presumably not worth spending too much computer time since this approximation has an unknown systematic error which does not allow for any reliable comparison with experiment in the end.

3 Dynamical Wilson Twisted Mass Simulations

The results discussed in the previous section are extremely encouraging if one thinks of simulations with dynamical quarks. Since the twisted mass parameter μ regulates the determinant, the simulations are expected to run very smoothly and light pseudo scalar masses of $m_{\rm PS} < 300$MeV ought to be reachable. Our collaboration decided therefore to start a scaling test for dynamical Wilson twisted mass fermions also for the case of two flavours of *dynamical fermions*. As in the quenched approximation, we had the expectation that the pion mass in its role as a Goldstone particle can be made as small as required from the experimental data and that the only obstacle in doing so ought to be the lack of computer resources given the algorithms that exist presently.

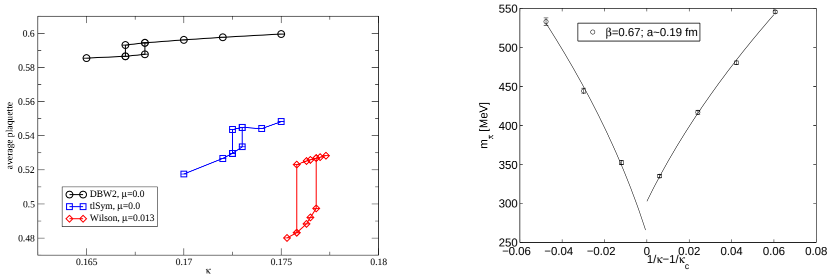

Figure 4. Left: Hysteresis curves for different gauge actions. Right: Non-vanishing minimal pseudo scalar mass in comparison to the predicted behaviour of chiral perturbation theory.

This expectation is guided by the continuum picture, where we have a jump of the scalar condensate at zero quark mass with the associated zero pseudo scalar mass as a result of the Goldstone theorem applied to the spontaneous breaking of chiral symmetry in QCD. This picture implies that the point of zero pseudo scalar mass is approached in a completely smooth way when the quark mass is lowered. To our surprise, we found that this picture fails completely! We refer to refs.[25–28] for a detailed account of this work. Instead of such a smooth behaviour, we found signs of rather strong first order phase transitions manifesting themselves in hysteresis effects, as known e.g. in magnetic systems, and long-living metastabilities with co-existing states. In fig. 4 we show such hysteresis effects employing different gauge actions demonstrating that the strength of the hysteresis and hence the strength of the first order phase transition depends strongly on the choice of the gauge action. Although such hysteresis effects are only first and somewhat naive indicators of the existence of a first order phase transition, in a number of works we studied the phenomenon in more detail and could indeed establish the existence of the first order phase transition.

Maybe, it is true that lattice QCD is already a rather old and mature field and almost nothing really new can be discovered. So it holds also for the case at hand: in a paper by Sharpe and Singleton[29] already in 1998, using the tool of lattice chiral perturbation theory the possibility of such a first order phase transition has been discussed and several properties of the phase transition were computed. The most remarkable and important of these properties is *that the pseudo scalar mass cannot reach zero, but only a certain minimal value*. In fig. 4 (right) we demonstrate this effect which shows up most clearly by the fact that the pseudo scalar masses from the positive and negative quark mass side intersect before reaching zero. We show also the anticipated behaviour from chiral perturbation theory[21,30,20,31–33] as the solid lines.

4 Conclusion

In this project, our collaboration has performed a detailed investigation of Wilson twisted mass fermions at full twist. The work has been presented at several international symposia and workshops and summaries of our work can be found in refs.[34,28,35]. In the quenched approximation, we have verified that maximally twisted Wilson fermions indeed lead to an

O(a)-improvement of physical observables leaving even O(a^2) effects small when the right definition of the critical quark mass is chosen.

For dynamical fermions, we could establish that for values of the lattice spacing relevant for a continuum extrapolation, we hit the phenomenon of a first order phase transition with a non-zero and moreover large value of a minimal pseudo scalar mass. Although this phenomenon is in accordance with results from chiral perturbation theory, it came somewhat a surprise. Anyhow, the phenomenon of this first order phase transition needed to be clarified before a large scale dynamical simulation could be started. Our collaboration has performed a detailed study of this question using numerical simulations and analytical techniques from chiral perturbation theory. As a result, we now have for the first time a comprehensive understanding of the lattice QCD phase diagram and the properties of the first order phase transition, see the report of the NIC research group elementary particle physics in these proceedings for a generic picture of the Wilson lattice QCD phase diagram.

As a main consequence of this work, we now know the action and the parameters where dynamical simulations can be performed without being affected by the first order phase transition. This is then the starting point for a detailed scaling study of Wilson twisted mass QCD also in the dynamical case. First simulations in this direction have already been started. Given the considerable algorithmic improvements obtained recently by our collaboration[36] and also by others[37], such simulations are realistic with present computer technology.

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